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Hall mobilities in GaN_xAs_{1-x}

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In this work we report a systematic study of the electron and hole mobilities of GaN_xAs_{1-x} alloys with different dopants (Zn, Te) and carrier concentrations (10^{17}-10^{19} cm^{-3}). We found a very slight reduction of the hole mobility in p-GaN_xAs_{1-x} compared to p-GaAs, indicating that for small N contents (~1.6%) the valence band is not affected by the N incorporation. In a striking contrast, incorporation of even small amounts of N leads to an abrupt reduction of the electron mobility in n-GaN_xAs_{1-x}. We further show that the processes that limit the mobility in GaN_xAs_{1-x} can be explained by the band broadening and the random field scatterings. Considering these two scattering mechanisms we calculated the dependence of electron mobilities on electron concentration as well as on N composition in GaN_xAs_{1-x}. The calculations agree reasonably well with experiment data of maximum electron mobilities with alloy composition.

1 Introduction Dilute nitride alloys have been studied for over a decade [1], due to their unusual physical properties and their technological potential for optoelectronic devices. These materials belong to the so-called highly mismatched alloys (HMAs), in which elements with very different electronegativity and/or size are alloyed to form a new class of semiconductors [2]. GaN_xAs_{1-x} with a small fraction of As replaced with N, is a very remarkable example of HMA. The higher electronegativity of N produces drastic changes in the band structure of GaAs, which influences its optical and electrical properties. Specifically, N interaction with the conduction band of GaAs leads to a reduction of the fundamental bandgap [3], an increase in the conduction band effective mass [4] and greatly improved the electrical activation of donors [5].

The salient feature of GaNAs alloys is the splitting of the conduction band due to the anticrossing interaction of the localized As states and the GaAs conduction band states. The splitting is described by the band anticrossing (BAC) model [6]. This model effectively predicts the properties of the alloy after the split, and describes the dispersion relation of the new bands, $E_+(k)$ and $E_-(k)$. The resulting structure is typical of a multiband semiconductor, which can be used for high efficiency solar cells [7].

Despite years of extensive studies only a very limited effort has been directed towards understanding of the transport properties of the GaNAs alloy system [8-15]. It has been shown that mobility in the $In_yGa_{1-y}N_xAs_{1-x}$ is limited mainly by two scattering mechanisms: the band broadening scattering (BBS) and the random field scattering (RFS) [3]. The former is deduced from the BAC model, and the later is a consequence of the random arrangement of the N impurities in the GaAs lattice, which produces a smooth field that is the source of scattering [16]. The aim of this paper is to study the electron and hole mobilities in GaN_xAs_{1-x}, and to propose a model based on these two mechanisms that can explain the mobility behavior with temperature, N concentration and carrier concentration.

2 Experimental Both p and n type GaN_xAs_{1-x} thin films doped with Zn and Te, respectively were grown by organometallic vapour phase epitaxy (OMVPE) using Dimethylhydrazine (DMHz) at a growth temperature of 600 °C. N composition in these films was estimated to be ~1.6% by x-ray diffraction and bandgap measured by photoreflectance. Hall effect measurements were performed in a homemade cryostat from liquid-He temperature to room temperature using the van der Pauw configuration.

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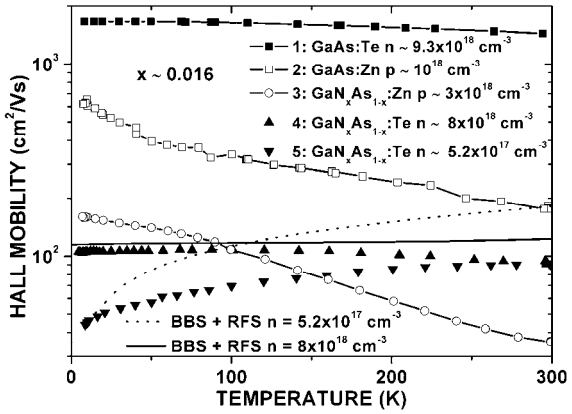

Figure 1 Hall mobility vs. temperature of GaAs and GaN_xAs_{1-x} samples. BBS+RFS model is applied for the Te doped GaN_xAs_{1-x} samples with x = 0.016.

3 Results and discussion Figure 1 shows the Hall mobility measured for 5 representative samples. Mobilities of GaN_xAs_{1-x} samples are always lower than mobilities of the GaAs samples of the same type. The slight reduction of the mobility in the p-type GaN_xAs_{1-x} samples can be explained by the scattering produced by the N atoms, since for small N contents the valence band is not affected by alloying of GaAs with GaN [2, 3]. In the case of the n-type samples, the considerable decrease of the mobility is not only caused by this mechanism. Additional contribution to the reduction of the Hall mobility comes from a change of the dispersion relation E_(k) and from a large increase of the electron effective mass [3]. It is also interesting to note that although sample 4 has more than 15 times higher carrier concentration than sample 5, they have very similar room temperature mobility. However it should be also noted that the temperature behavior of Hall mobility is completely different in these two samples. This indicates that different scattering mechanisms limit the electron mobility of GaN_xAs_{1-x}, depending on the carrier concentration of the sample, the N concentration, and the temperature.

Initial estimates have shown that the traditional scattering mechanisms, such as alloy scattering [17], neutral impurity scattering [18] or deformation potential scattering [19], are negligible in n-GaN_xAs_{1-x}. Only the ionized impurity scattering [20] should be considered for very high carrier concentration ($n > 10^{19}$ cm^{-3}).

The BBS is dependent on the strength of the hybridization of the states in the E_(k) band that could limit the lifetime of carriers, and it can be estimated through the BAC model. Details of this model is described in Ref. [2] and [3]. In this model the mobility can be expressed as:

$$\mu = \frac{e\tau(k_F)}{m_-(k_F)} \approx \frac{e\hbar}{m_-(k_F)\Gamma_-(k_F)} \quad (1)$$

where e is the electron charge, $\hbar$ is the reduced Planck constant, m_ is the mass of the carriers in the E_(k) band, k_F is the Fermi surface wavevector and Γ_ is the broadening of the dispersion relations [3]. For the calculation of equation (1) we assumed a parabolic model for the GaAs conduction band, choosing for the conduction band minimum the Varshni empirical model and a linear behavior with temperature for the effective mass [21]. The prefactor for the energy broadening β [2] was treated as a fitting factor and a value of 0.3 was chosen, very close to the 0.22 estimated by Wu *et al*. for InGaNAs [2].

To model the RFS, the onset of a smooth field has to be considered. Depending on the sign of the Fermi level, two different formulas are used [16]:

$$\mu = \frac{3\pi}{8} e \sqrt{\frac{E_F}{2m_-(k_F)\Psi_2}}, \quad E_F > 0 \quad (2)$$

$$\mu = e \sqrt{\frac{\pi kT}{2m_-(k_F)\Psi_2}}, \quad E_F < 0 \quad (3)$$

where k is the Boltzmann constant, T is the absolute temperature and Ψ_2 is the mean square of the gradient of the fluctuations of the potential energy of an electron in the random field. In the calculation of the Fermi level, integration converges in a small range of energy [2, 3]. Defining a cubic volume inside the lattice, where the standard deviation of N concentration can be estimated, one can use the BAC model to evaluate the magnitude of the variation of the field. Relating this variation to the average distance between N atoms, and multiplying by a constant fitting factor, we estimated Ψ_2 to be in the range of $10^4 \le \Psi_2^{1/2} \le 10^5$ eV/cm for a slow varying field [22]. Matthiessen`s rule is used to calculate the combined effect of BBS and RFS.

Figure 1 includes the calculations for Hall mobility of samples 4 and 5 with varying temperature, using equation (1) to evaluate the BBS, and Eqs. (2) and (3) to estimate the RFS. As is seen in Fig. 1 the calculations well reproduce the magnitude as well as the temperature dependence of the mobility. The only difference between samples 4 and 5 is the carrier concentration, and that requires the use of equation (2) for sample 5, in which Fermi level is negative, and equation (3) for sample 4, in which Fermi level is positive. The BBS seems to dominate at higher electron concentration when the Fermi level is located closer to the N-level (see Fig. 2), whereas the RFS plays a more important role at low concentrations and lower temperatures, when the potential fluctuations are comparable to or larger than the average electron energy. In Ref. [15] temperature behavior of GaN_xAs_{1-x} mobility is modeled, but this model does not account for the different temperature dependences presented in Fig. 1.

Figure 2 shows the calculated carrier concentration dependence of the mobility for different N concentrations, at

300 K. The trend is different from that reported by Shan *et al.* [3], but it is consistent with experimental results reported in the literature [11, 24, 26]. The saturation of the mobility at low carrier concentration has been previously reported in Ref. [11], but in this case the low carrier concentration mobility saturates at about an order of magnitude higher value. Also, the calculations presented in Ref. [8] for x=0.02 give mobilities higher than our prediction.

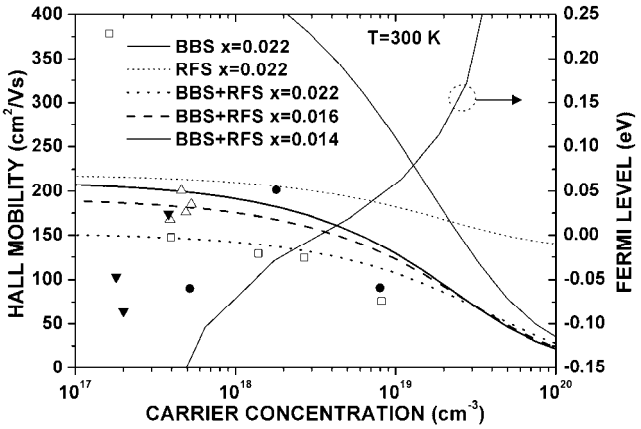

Figure 2 Hall mobility as a function of carrier concentration. Experimental results (0.014<x<0.022) from: (□) Ref. [11], (▼) Ref. [24], (△) Ref. [26], (●) our measurements. Fermi level was calculated at room temperature for x=0.016.

Variation of Fermi level with carrier concentration for x=0.016 is also plotted in Fig. 2. It is worth noting that equations (2) and (3) are only valid in the range $|E_F| > kT$ [16], therefore, strictly speaking, at T=300 K our model might not be valid in the carrier concentration range $2x10^{18}$-$6x10^{18}$ cm^{-3}.

Finally, Fig. 3 shows results of the N concentration dependent mobility combining the BBS and RFS. All the experimental data points are either below or very close to our calculations, confirming the validity of the model. Calculations by Fahy and O'Reilly [10] and Vaughan and Ridley [11] are also shown in Fig. 3. Although the actual mobility values calculated using the different models differ significantly all of the calculations reproduce a much weaker dependence on the N concentration observed at high N contents. Similar behavior was also found previously in [14] and [15].

4 Conclusions Two different scattering mechanisms are proposed to explain the behavior of Hall mobility for n-type GaN_xAs_{1-x}. We have found that band broadening scattering is dominant at high electron concentrations whereas random field scattering prevails at low electron concentrations and at lower temperatures. On the other hand, random field scattering is more important in the high N concentration range. These two processes describe reasonably well our experimental results and those reported in the literature.

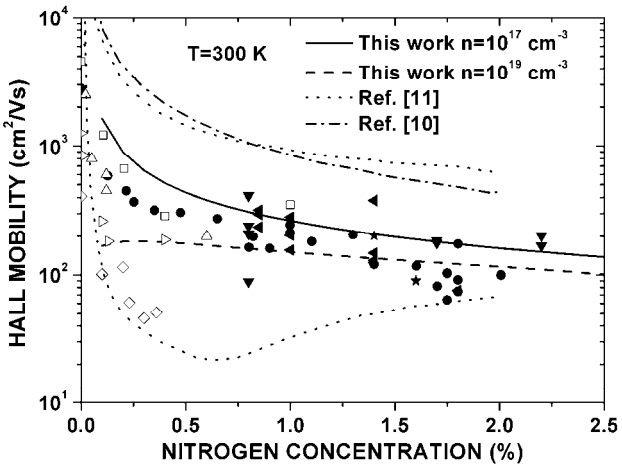

Figure 3 Hall mobility as a function of N concentration. (◀) Ref. [11], (△) Ref. [12], (□) Ref. [14], (▷) Ref. [23], (●) Ref. [24], (◇) Ref. [25], (▼) Ref. [26], (★) our measurements.

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